



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 12:39 PM EDT

PDB ID : 5IZM
Title : The crystal structure of human eEFSec in complex with GDPNP
Authors : Dobosz-Bartoszek, M.; Otwinowski, Z.; Simonovic, M.
Deposited on : 2016-03-25
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

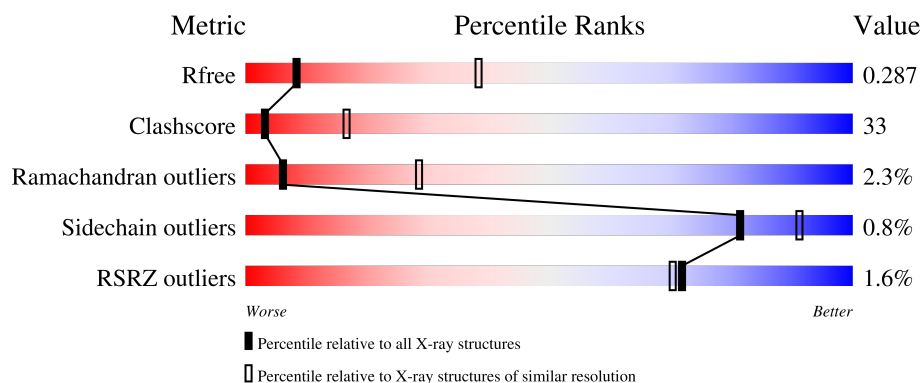
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	616	
1	B	616	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	Se	0	1	0
			3147	2026	544	554	9	14			
1	B	495	Total	C	N	O	S	Se	0	0	0
			3419	2212	579	604	9	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP P57772
A	-18	GLY	-	expression tag	UNP P57772
A	-17	SER	-	expression tag	UNP P57772
A	-16	SER	-	expression tag	UNP P57772
A	-15	HIS	-	expression tag	UNP P57772
A	-14	HIS	-	expression tag	UNP P57772
A	-13	HIS	-	expression tag	UNP P57772
A	-12	HIS	-	expression tag	UNP P57772
A	-11	HIS	-	expression tag	UNP P57772
A	-10	HIS	-	expression tag	UNP P57772
A	-9	SER	-	expression tag	UNP P57772
A	-8	SER	-	expression tag	UNP P57772
A	-7	GLY	-	expression tag	UNP P57772
A	-6	LEU	-	expression tag	UNP P57772
A	-5	VAL	-	expression tag	UNP P57772
A	-4	PRO	-	expression tag	UNP P57772
A	-3	ARG	-	expression tag	UNP P57772
A	-2	GLY	-	expression tag	UNP P57772
A	-1	SER	-	expression tag	UNP P57772
A	0	HIS	-	expression tag	UNP P57772
A	1	MSE	-	expression tag	UNP P57772
B	-19	MSE	-	initiating methionine	UNP P57772
B	-18	GLY	-	expression tag	UNP P57772
B	-17	SER	-	expression tag	UNP P57772
B	-16	SER	-	expression tag	UNP P57772

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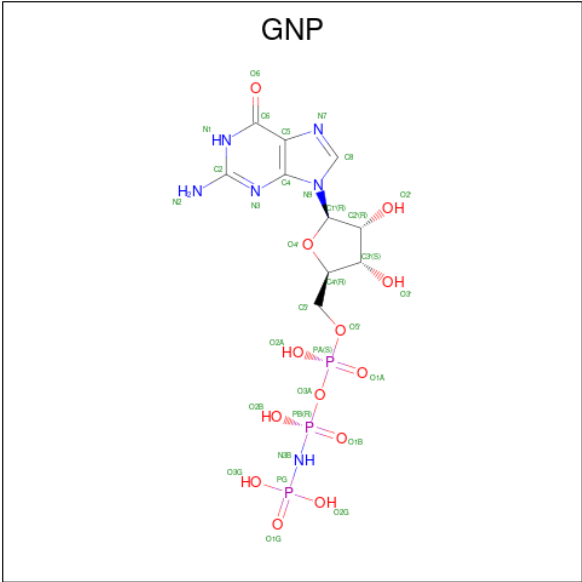
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P57772
B	-14	HIS	-	expression tag	UNP P57772
B	-13	HIS	-	expression tag	UNP P57772
B	-12	HIS	-	expression tag	UNP P57772
B	-11	HIS	-	expression tag	UNP P57772
B	-10	HIS	-	expression tag	UNP P57772
B	-9	SER	-	expression tag	UNP P57772
B	-8	SER	-	expression tag	UNP P57772
B	-7	GLY	-	expression tag	UNP P57772
B	-6	LEU	-	expression tag	UNP P57772
B	-5	VAL	-	expression tag	UNP P57772
B	-4	PRO	-	expression tag	UNP P57772
B	-3	ARG	-	expression tag	UNP P57772
B	-2	GLY	-	expression tag	UNP P57772
B	-1	SER	-	expression tag	UNP P57772
B	0	HIS	-	expression tag	UNP P57772
B	1	MSE	-	expression tag	UNP P57772

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

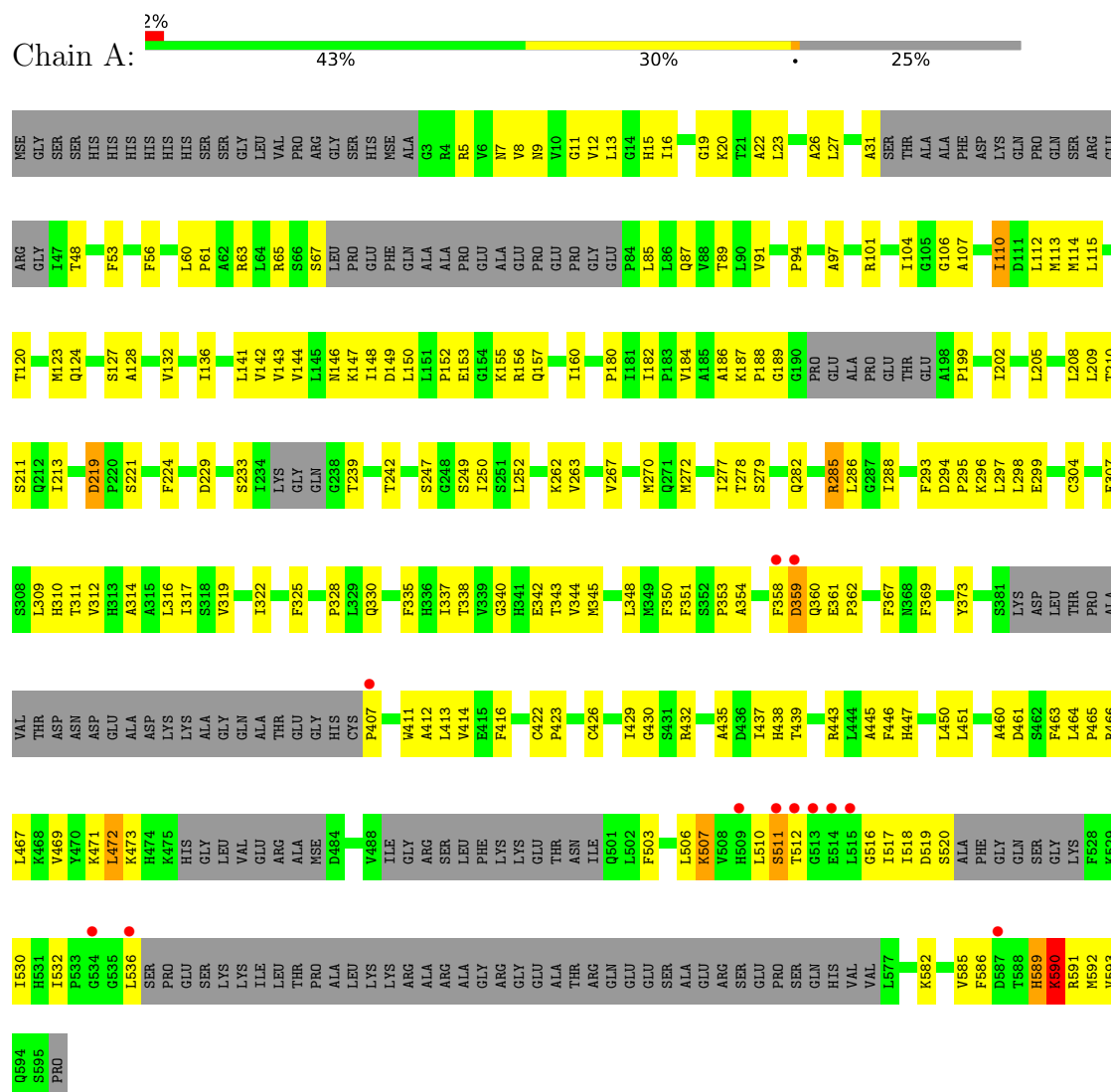


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Selenocysteine-specific elongation factor



ALA	GLU	ARG	SER	GLU	PRO	S572	Q573	H574	V575	L579	T580	F581	K582	V585	F586	D587	T588	H589	M592	V593	Q594	S595	PRO																																	
1489	G490	R491	S492	L493	F494	LYS	LYS	E497	T498	N499	L500	Q501	F503	V504	L510	S511	T512	G513	L518	D519	S520	G523	GLN	SER	GLY	K527	F528	K529	L530	H531	L532	P533	L544	THR	PRO	ALA	ALA	ALA	LEU	LYS	LYS	ARG	ALA	ARG	ALA	ALA	GLY	ARG	GLY	GLU	THR	ARG	GLN	GLU	GLU	SER
LYS	ALA	GLY	GLN	ALA	THR	GLU	GLY	HIS	CYS	P407	V414	V420	T421	L425	C426	L427	V428	L429	G430	S431	R432	L433	D434	A435	ASP	ILE	H438	C442	R443	L444	A445	F446	H447	L450	G453	V459	A460	L464	P465	V470	K471	L472	G477	L478	V479	E480	N483									
E320	K321	I322	P323	L324	F325	L329	Q330	T331	I337	T338	V344	M345	G346	R347	L348	M349	F350	F351	G352	P353	A354	P355	F358	D359	Q360	E361	P362	N368	F369	S370	Q371	E372	Y373	E377	Q378	Y379	L380	S381	LYS	ASP	LEU	THR	PRO	ALA	VAL	THR	ASP	ASN	ASP	GLU	ALA	ASP	LYS			
T217	P220	P223	F224	L225	M226	F232	F233	T239	V240	M241	T245	L246	S247	I250	S251	E257	T258	P259	A260	L261	K265	K266	V267	M270	Q271	M272	L277	A280	L286	T291	Q292	F293	D294	P295	K296	L297	L298	C304	L309	H310	T311	V312	V319													
V132	I133	Q134	Q135	I136	V144	L145	N146	K147	I148	D149	L150	L151	P152	E153	GLY	LYS	R156	I160	D161	R177	G178	A179	P180	I181	I182	P183	V184	K187	P188	G189	G190	PRO	GLU	ALA	PRO	GLU	THR	GLU	D111	L112	M113	M114	L115	T120	K121	G122	M123	Q124	T125	Q126	S127	A128	E129	G130	L131	
MSE	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	GLN	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MSE	ALA	R4	N7	V8	N9	V10	G11	V12	L13	G14	H15	I16	G19	K20	T21	A22	L23	A24	L27	A31	SER	THR	ALA	ALA	PHE	ASP	LYS	GLN	PRO	GLN	SER	ARG	GLU	ARG		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	92.32Å 112.40Å 327.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 3.40 46.16 – 3.38	Depositor EDS
% Data completeness (in resolution range)	78.4 (46.16-3.40) 84.9 (46.16-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.235 , 0.285 0.236 , 0.287	Depositor DCC
R_{free} test set	1114 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	6632	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/3193	0.77	12/4335 (0.3%)
1	B	0.37	0/3467	0.72	9/4708 (0.2%)
All	All	0.39	0/6660	0.75	21/9043 (0.2%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LYS	CB-CA-C	-7.40	95.59	110.40
1	B	225	LEU	N-CA-CB	-6.58	97.25	110.40
1	A	592	MSE	CB-CA-C	-6.37	97.66	110.40
1	B	445	ALA	CB-CA-C	-6.24	100.75	110.10
1	A	511	SER	N-CA-C	6.23	127.83	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3147	0	2871	206	0
1	B	3419	0	3163	219	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	13	7	0
3	B	32	0	13	2	0
All	All	6632	0	6060	424	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 424 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:MSE:CB	1:B:286:LEU:HD23	1.20	1.64
1:B:272:MSE:CE	1:B:286:LEU:HD21	1.17	1.58
1:B:272:MSE:CG	1:B:286:LEU:HD23	1.45	1.43
1:B:272:MSE:HB2	1:B:286:LEU:CD2	1.55	1.37
1:B:272:MSE:CB	1:B:286:LEU:CD2	2.05	1.34

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/616 (72%)	350 (79%)	81 (18%)	10 (2%)	6	28
1	B	475/616 (77%)	377 (79%)	87 (18%)	11 (2%)	6	28
All	All	916/1232 (74%)	727 (79%)	168 (18%)	21 (2%)	6	28

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	LYS
1	A	296	LYS

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Mol	Chain	Res	Type
1	A	359	ASP
1	A	439	THR
1	A	511	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/507 (55%)	276 (99%)	2 (1%)	84	92
1	B	312/507 (62%)	309 (99%)	3 (1%)	76	88
All	All	590/1014 (58%)	585 (99%)	5 (1%)	81	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ILE
1	A	507	LYS
1	B	233	SER
1	B	286	LEU
1	B	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	B	7	ASN
1	B	9	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GNP	B	1002	2	29,34,34	3.18	10 (34%)	33,54,54	2.18	9 (27%)
3	GNP	A	1002	2	29,34,34	3.18	10 (34%)	33,54,54	2.18	9 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	B	1002	2	-	2/14/38/38	0/3/3/3
3	GNP	A	1002	2	-	5/14/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	GNP	PG-O1G	10.21	1.62	1.46
3	A	1002	GNP	PG-O1G	10.19	1.62	1.46
3	A	1002	GNP	PB-O1B	10.17	1.62	1.46
3	B	1002	GNP	PB-O1B	10.14	1.62	1.46
3	B	1002	GNP	C5-C6	-4.57	1.33	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	GNP	N3-C2-N1	-5.89	119.36	127.22
3	A	1002	GNP	N3-C2-N1	-5.89	119.36	127.22
3	A	1002	GNP	C2-N3-C4	4.67	120.69	115.36
3	B	1002	GNP	C2-N3-C4	4.64	120.66	115.36
3	A	1002	GNP	O1B-PB-N3B	-4.54	105.09	111.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GNP	PB-N3B-PG-O1G
3	A	1002	GNP	PG-N3B-PB-O1B
3	B	1002	GNP	PB-N3B-PG-O1G
3	B	1002	GNP	PG-N3B-PB-O1B
3	A	1002	GNP	O4'-C4'-C5'-O5'

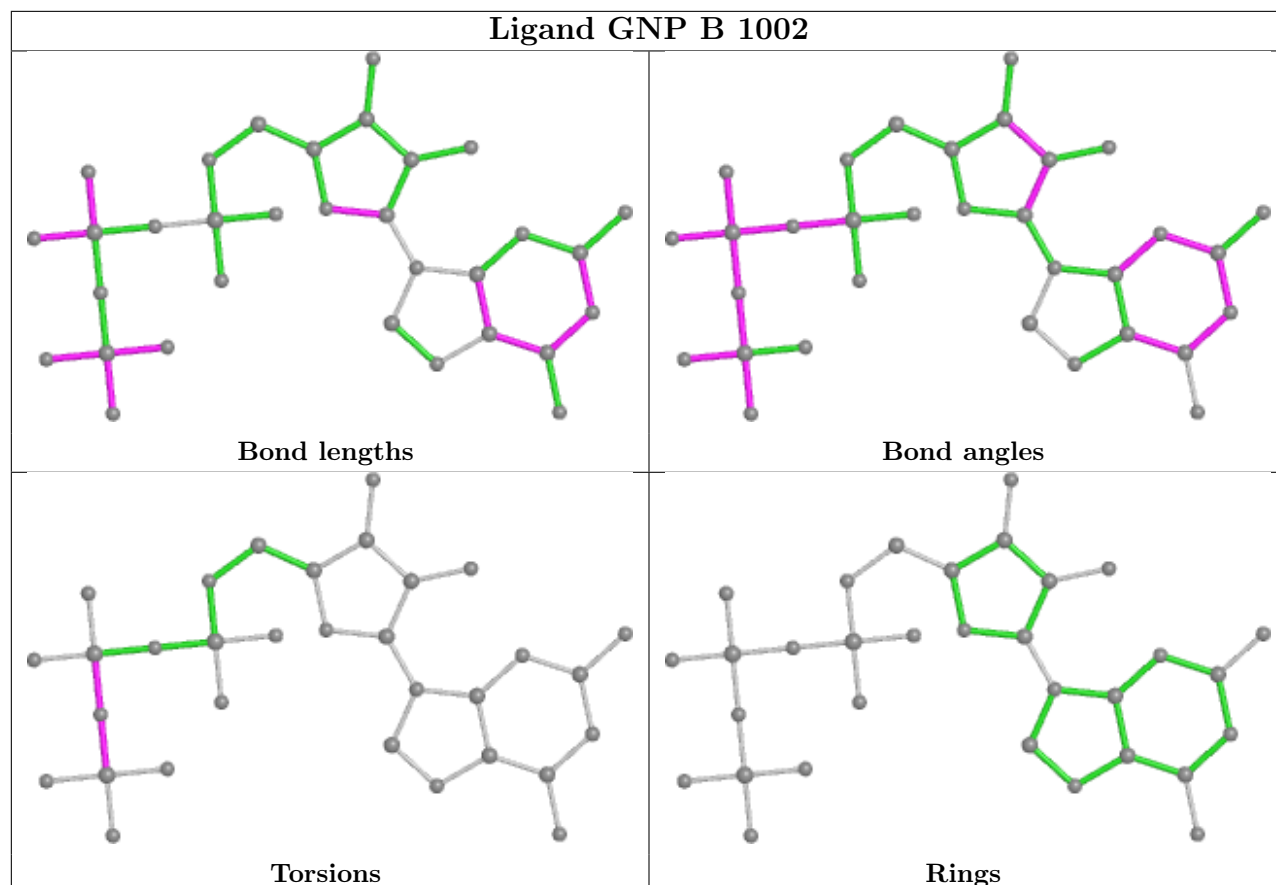
There are no ring outliers.

2 monomers are involved in 9 short contacts:

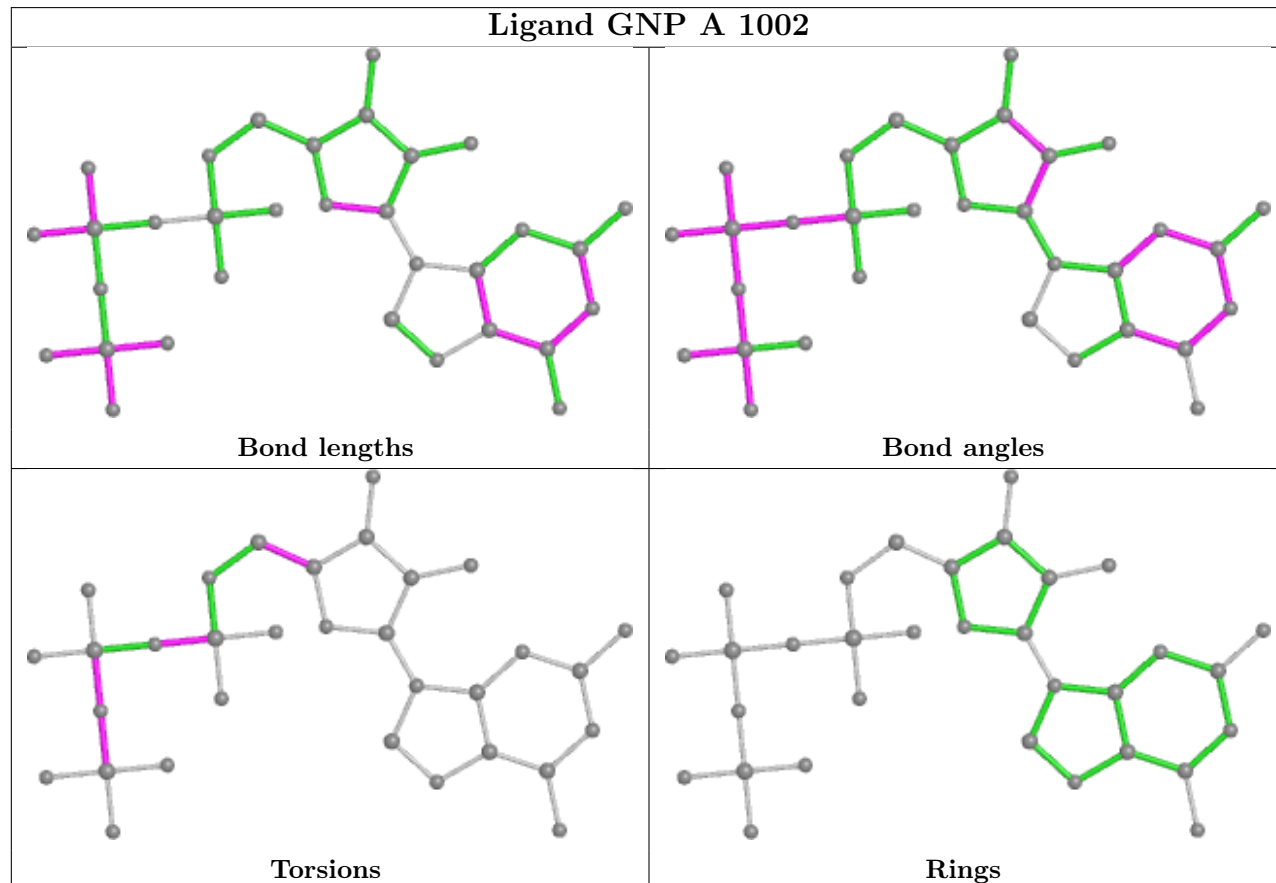
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	GNP	2	0
3	A	1002	GNP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP B 1002



Ligand GNP A 1002



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	446/616 (72%)	-0.03	12 (2%) 54 53	6, 31, 70, 104	0
1	B	480/616 (77%)	-0.19	3 (0%) 89 89	8, 28, 55, 76	0
All	All	926/1232 (75%)	-0.11	15 (1%) 72 70	6, 30, 64, 104	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	ASP	3.2
1	A	514	GLU	2.8
1	A	536	LEU	2.8
1	A	515	LEU	2.6
1	A	534	GLY	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

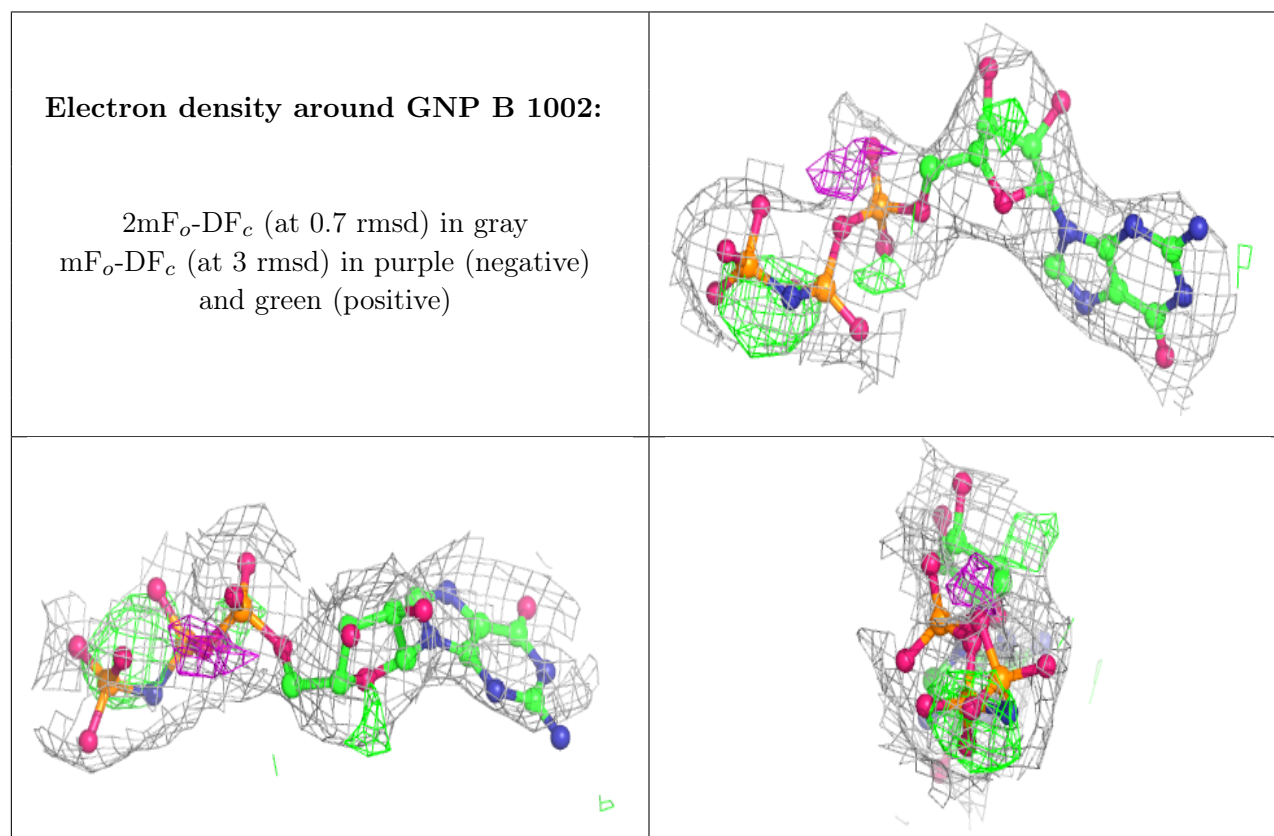
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

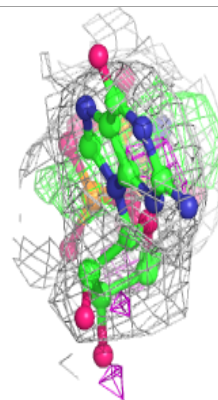
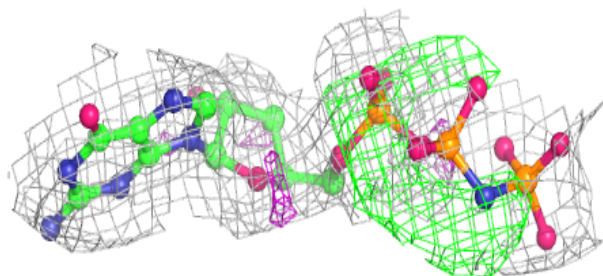
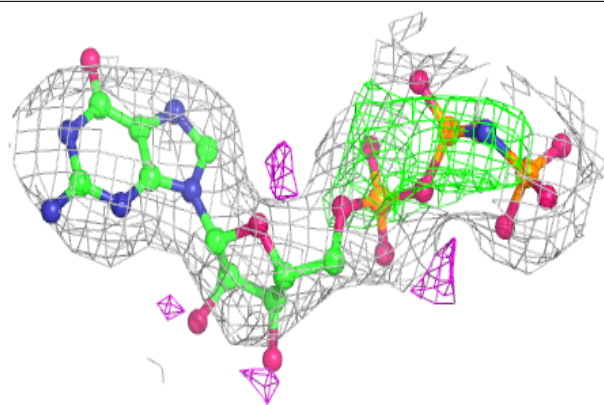
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GNP	B	1002	32/32	0.89	0.26	24,54,66,96	0
3	GNP	A	1002	32/32	0.90	0.27	17,47,78,96	0
2	MN	A	1001	1/1	0.97	0.07	16,16,16,16	0
2	MN	B	1001	1/1	0.97	0.13	15,15,15,15	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around GNP A 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.